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Magnon caustics in face centered cubic ferromagnets

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Abstract. Caustic phenomenon in magnon propagation picture in face centered cubic lattice is investigated. The employed model takes into account the Heisenberg exchange interaction between an atom's spin and it's nearest and next nearest neighbors. Caustic directions are defined by exploring the corresponding dispersion relations. On the basis of face centered cubic lattice of EuS ferromagnet, such singular peculiarities are investigated for different Heisenberg exchange parameters. Magnon energy regions where the caustics can be observed are defined together with the caustic directions in characteristical crystallographic planes $\{100\}$ and $\{110\}$. It was obtained that caustics can be observed if the magnon frequency is about hundreds of gigahertz, and the widths of the caustic direction regions, that are determined by the magnon frequencies, are of the order of dozens of degrees.

1. Introduction

In the present paper, the problem of magnon caustics formation in ferromagnets with cubic structure is studied. The paper is devoted mainly to the ferromagnets with face centered cubic (FCC) lattice. An example of material of this type is EuS ferromagnet. In addition, the possibilities of caustics observation in ferromagnets with other cubic structures (simple cubic (SC) and body centered (BCC)) are considered. The properties of spin waves depend on the propagation direction in ferromagnets with cubic lattices, and the group velocity vector and wavevector are noncollinear. The preferred directions of wave propagation appear therefore in such systems. For some FCC-ferromagnets the magnon flow intensity increases sharply along a specific direction, this direction corresponds to the spin wave caustic. During recent years, the magnon caustic phenomenon has been being the topic of interest because of it's possible practical applicatons; e.g. in spin signals multiplexing [1]. One of the materials promising for spin wave caustics observation is EuS, which has FCC lattice structure. The magnetic properties of EuS are well-described in the framework of Heisenberg exchange hamiltonians. Note that Eu^{2+} ions in this compound have the spin states $^8S_{7/2}$ when electronic orbital moment is absent ($L = 0$, $S = J = 7/2$). The magnetic anisotropy in this compound is about 30 Oe and it can be neglected [2] in calculations therefore. In our previous papers, the anisotropy of magnon propagation in EuS has already been described [3], but the goal of this paper is the investigation of a fine feature of anysotropy, namely, the dependencies of the caustic directions on the magnon energy. This problem would be important, for instance, due to it's possible practical applications for overcoming the challenges which complementary metal-oxide-semiconductor-based devices are facing today [1].

2. Spin wave spectrum

Let us consider the spin wave properties in EuS. It is a ferromagnetic material with FCC lattice, and its spin-wave Hamiltonian is written as [4, 5]

$$\mathcal{H} = -J_1 \sum_{j,\delta_1} S_j S_{j+\delta_1} - J_2 \sum_{j,\delta_2} S_j S_{j+\delta_2} \tag{1}$$

In (1) the first and second terms describe exchange interaction of a chosen atom's spin with its first and second neighbors, respectively. The sum over j includes all atoms of the crystal and the sums over δ_1 and δ_2 take into account all the nearest and next nearest neighbors of atom j. External magnetic field is assumed to be zero in this paper. Generally, the term responsible for magnetic anisotropy has to be included in the Hamiltonian, but as it was mentioned, the anisotropy can be neglected for the EuS ferromagnet. Furthemore, the external magnetic field and the anisotropy field induce the emersion of a gap in the magnon spectrum, but do not change its angular dependences [3]. In this paper, we are interested in the dependence of the spin wave properties on the propagation directions only. Thus, taking into account anisotropy terms and the external magnetic field produces some complexity of the calculation, but does not effect the principal results. These terms are excluded from the consideration therefore. The magnon energy is obtained from (1) employing the standard Hamiltonian diagonalization method [6]:

$$\hbar\omega(\mathbf{q}) = 2S\{J_1 \sum_{j,\delta_1}(1 - e^{-i\mathbf{q}\cdot\mathbf{r}_{j+\delta_1}}) + J_2 \sum_{j,\delta_2}(1 - e^{-i\mathbf{q}\cdot\mathbf{r}_{j+\delta_2}})\} \tag{2}$$

The summation over neighboring atoms in FCC lattice leads to the following dispersion relation:

$$\begin{aligned}\tilde{\omega}(\mathbf{q}) = 4\left\{3 - \cos\frac{aq_x}{2}\cos\frac{aq_y}{2} - \cos\frac{aq_y}{2}\cos\frac{aq_z}{2} - \cos\frac{aq_x}{2}\cos\frac{aq_z}{2}\right\} + \\ +2\xi\{3 - \cos aq_x - \cos aq_y - \cos aq_z\}\end{aligned} \tag{3}$$

Here, q_i is the wave vector components, parameter a is the lattice period, J_1 and J_2 are the parameters of Heisenberg exchange interaction between chosen atom's spin and its next and next nearest neighbors, S is the spin of atoms, the frequency is given in dimensionless form $\tilde{\omega} = \omega(\mathbf{q})/\omega_e$, where $\omega_e = 2SJ_1/\hbar$, and $\xi = J_2/J_1$ characterizes the ratio of exchange coupling constants. The EuS parameters are known: $S = 7/2$, and $\omega_e/2\pi \approx 34.4\,\mathrm{GHz}$, $J_1 = 0.236\,\mathrm{K}$, $J_2 = -0.118\,\mathrm{K}$ [4, 5], $\xi = J_2/J_1 \approx -0.5$.

The dispersion relation (3) demonstrates the anisotropic properties of the waves: the frequency $\tilde{\omega}$ depends on the direction of the wavevector $\mathbf{q}$. The constructive characteristic of this anisotropy was introduced in [7]. Within applied approach, the authors calculated the value of phonon amplification factor A, which is equal to the relation of the flow intensity in the crystal to the intensity of an isotropic flow. This approach was generalized to magnon case in [8]. An important feature of the approach is the possibility of caustics investigation. In this context, the caustic is determined as the lattice direction, where the amplification factor value tends to infinity. Another important feature of the theory [7] is as follows. The amplification factor is determined simply through the properties of the constant energy surface, namely $A \sim 1/|K|$, where K is the Gaussian curvature. Thus, the points of zero Gaussian curvature determine the caustic directions. In present study Gaussian curvatures are investigated in two most important cross sections of the constant energy surfaces – $\{100\}$ and $\{110\}$ planes. These sections include characteristic directions [100], [110], and [111]. The surfaces are plotted in spherical coordinates (q, θ, ϕ). Cross sections $\{100\}$ and $\{110\}$ correspond to the value of ϕ equal to 0 and $\pi/4$, respectively. A picture illustrating focusing and caustic is given in the figure 1. Points of zero curvature (the concave part transforms into the convex one) correspond to the caustic directions. Focusing takes place in the [001] and [110] directions in the figure 1.

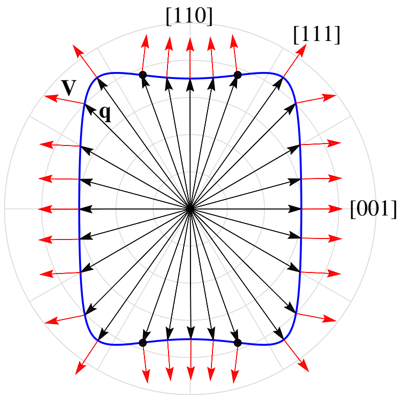

Figure 1. $\{110\}$ cross section of magnon constant frequency surface with $\tilde{\omega} = 5.4$ ($\omega/2\pi = 186\,\mathrm{GHz}$) and $\xi = -0.5$. Black arrows are the wavevectors and red arrows are the corresponding group velocity vectors. Bold points designate the points of zero Gaussian curvature.

3. Caustics in EuS

Let us start the investigation of caustics from a material with well known characteristics, namely the EuS ferromagnet. The only one parameter ξ of the spin wave spectrum (3) is equal to $\xi = -0.5$ for this case. According to the above mentioned method of focusing phenomenon investigation on the basis of the amplification factor, it is necessary to study the constant frequency surfaces $q(\theta,\phi)\Big|_{\omega=const}$. In this context, the principal crystallography planes $\{100\}$ and $\{110\}$ are studied, and the constant frequency surfaces are constructed. The amplification factor $A(\theta,\phi,\omega) = V_n/(Vq^2|K(\theta,\phi,\omega)|)$ is calculated for these planes. Here V_n is the component of the group velocity vector $\mathbf{V}$, perpendicular to the surface $\omega = const$, and $K(q,\theta,\phi)$ is the Gaussian curvature at the point with spherical coordinates (q,θ,ϕ). The result for the $\{100\}$ plane is shown in the figure 2. The angle ϕ is equal to 0 in this case, and the dependence on the angle θ is symmetric relative to $\theta = \pi/4$. For the small frequencies ($\tilde{\omega} = 3$, line 1) the amplification factor is a smooth function of θ, but it becomes a function with second order discontinuances for a large value of $\tilde{\omega}$ (see lines 2 and 3 in the figure 2). These angles of discontinuances determine the caustic directions. The caustics appear at the angle θ close to $\pi/4$ at the frequency $\tilde{\omega} \approx 4$ and their directions decrease almost to zero when $\tilde{\omega}$ increases up to $\tilde{\omega} \approx 6$. The dashed line in the figure 2 corresponds to $A = 1$, i. e. isotropic propagation of the waves. The parts of $A(\theta)$ lines above the dashed line denote the focusing of the waves, and the parts below – defocusing. Note that the $\{100\}$ plane becomes focusing ($A > 1$) for all θ if the frequency is small enough, and a defocusing region appears only for high frequency.

Note that in the case of EuS we have to restrict our consideration to $\tilde{\omega} = \tilde{\omega}_{max} = 6$ and $qa = 5.44$ due to the following reasons. It follows from dispersion relation (3) that if the wavenumber qa is less then 5.44, then the frequency $\tilde{\omega}$ is a monotonously increasing function of qa for any direction θ,ϕ, while for $qa > 5.44$ the function $\tilde{\omega}(qa)$ remains increasing for some direction and becomes decreasing for other. Thus, for the frequencies $\tilde{\omega} < 6$ the equation $\omega(q,\theta,\phi) = const$ with respect to q has the solution for any (θ,ϕ), while some directions becomes forbidden for $\tilde{\omega} > 6$. Note, that the caustic frequencies region for EuS is equal to $4 < \tilde{\omega} < 6$, that corresponds to the $\omega/2\pi \in (138; 206)\,\mathrm{GHz}$.

The similar situation occurs for the $\{110\}$ plane ($\phi = \pi/4$, $0 < \theta < \pi$): the curve $A(\theta)$ is a

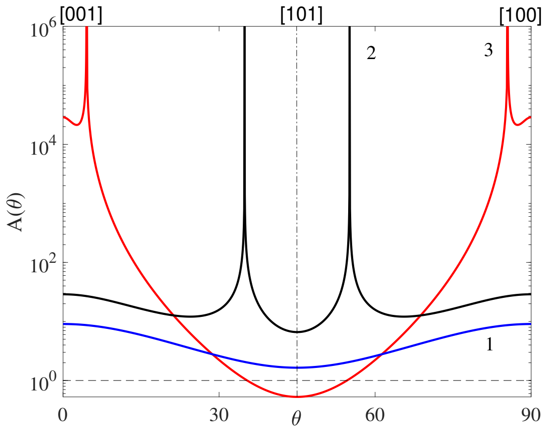

Figure 2. The dependence of amplification factor on the angle θ in $\{100\}$ plane in EuS ferromagnet. Line 1 corresponds to the frequency $\tilde{\omega} = 3$, line 2 refers to $\tilde{\omega} = 4.2$, and line 3 represents $\tilde{\omega} = 6$.

smooth function for small frequencies and demonstrates the caustic behavior for high frequencies. Investigation of the dependence of caustic directions on frequency is important for the practical applications of magnon caustics. The result is shown in the figure 3 (a) ($\{100\}$ plane) and (3) (b) ($\{110\}$ plane). Line 1 in the figure 3 represents the dependence of caustic angles θ_{cq} (for $\{100\}$ and $\{110\}$ plane) on the frequency. As it was mentioned above, wavevectors and group velocity vectors are non-collinear in the cubic lattices. The energy transfer is realized along the group velocity direction. Thus, it is important to know the caustic direction in the group velocity space. The dependencies of this direction on the frequency are shown by the lines 2 figure 3. In the $\{100\}$ plane, the caustic angles both in q- and V-spaces occupy the region $0 < \theta_c < \pi/4$, but the function $\theta_{cV}(\tilde{\omega})$ decreases faster than $\theta_{cq}(\tilde{\omega})$. Note that $\theta = 0$ corresponds to the direction [001] and $\theta = \pi/4$ – to the direction [101]. The situation differs for $\{110\}$ plane. The caustic angle in q-space is within the region $55^\circ \lesssim \theta_{cq} < 90^\circ$, while in V-space θ_{cV} is an increasing function of $\tilde{\omega}$ and occupies the region $90^\circ < \theta_{cV} \lesssim 110^\circ$. Note that angle $\theta = 90^\circ$ corresponds to [110] direction and $\theta > 90^\circ$ means that the caustic direction is negative with respect to [001] direction.

4. Caustics in FCC, BCC and SC lattices

The previous section was devoted to the investigation of caustic direction in the FCC lattice in the framework of the model that takes into account the exchange interaction of atom's spin with its nearest and next nearest neighbors. The ratio between the coupling constants was equal to $\xi = -0.5$, what corresponds to EuS ferromagnet. In this section the following questions are considered. (I) How the caustic picture transforms if the parameter ξ is varied in FCC lattice, and (II) what about caustic in a body centered and a simple cube lattices.

The answer for the question (I) is as follows. If the absolute value of coupling parameter ξ becomes smaller, then the caustic region becomes narrower and shifts to the high frequency region. A more interesting caustic picture is realized when $|\xi|$ becomes greater. In this case we deal with two effects. The caustic region becomes grater and shifts to the lower frequencies, and a region of multiple caustics appears. For instance, if $\xi = -0.7$, then (1) no caustic can be observed if $0 < \tilde{\omega} < 1.58$, (2) one caustic is realized in the region $1.58 < \tilde{\omega} < 2.45$, and (3) three caustic exist in the region $2.45 < \tilde{\omega} < 3.6$, where $\tilde{\omega}_{max} = 3.6$ is the maximum value of frequency for $\xi = -0.7$. The situation is shown in the figure 4. The first caustic branch

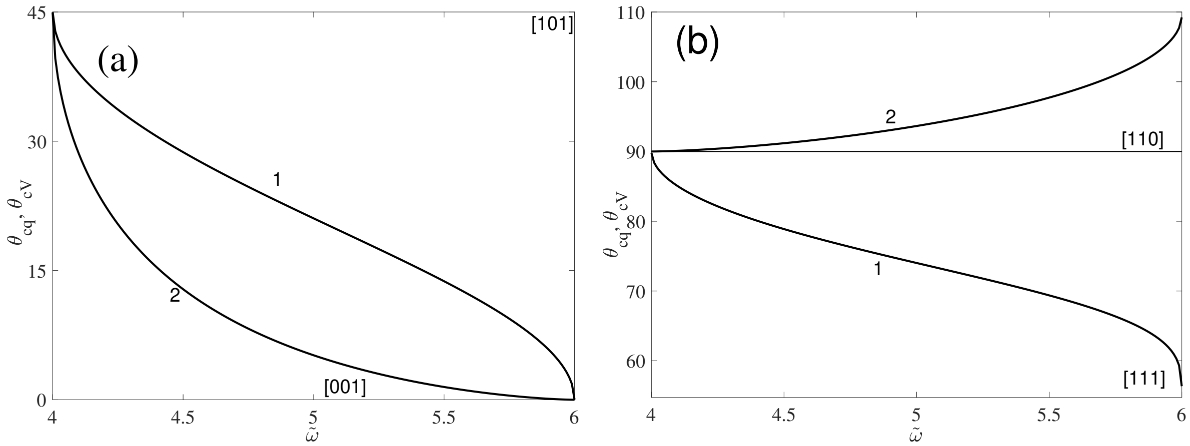

Figure 3. Dependencies of caustic directions on magnon frequency ($\tilde{\omega}$) for EuS lattice. $\theta_{cq}(\tilde{\omega})$ and $\theta_{cV}(\tilde{\omega})$ designate the caustic angles in reciprocal (1) and direct (2) spaces, respectively. (a) and (b) designate $\{100\}$ and $\{110\}$ cross-sections, respectively.

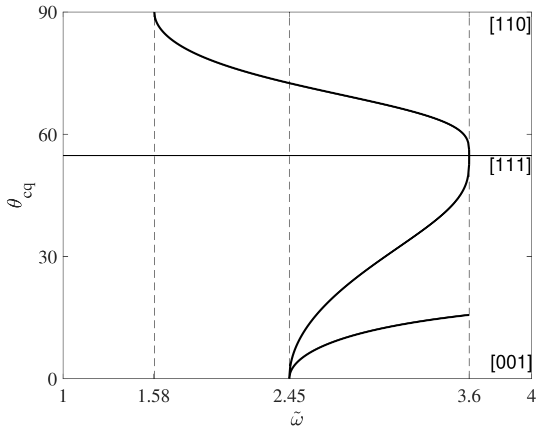

Figure 4. Dependence of caustic directions on magnon frequency ($\tilde{\omega}$) for FCC lattice with $\xi = -0.7$ in $\{110\}$ plane.

occurs at the frequency $\tilde{\omega} = 1.58$ and decreases with ω: $\theta_{cq}(1.59) = 90°$ and $\theta_{cq}(3.6) \approx 55°$. The second caustic branch appears at $\tilde{\omega} = 2.45$. It increases from $\theta_{cq} = 0$ and connects with the first branch at $\tilde{\omega} = \tilde{\omega}_{max}$. The third caustic branch also appears at $\tilde{\omega} = 2.45$ and increases from $\theta_{cq} = 0$ to $\theta_{cq} \approx 13°$. The results are compiled in the Table 1, where the frequency regions and corresponding caustic direction regions are presented for $\xi = -0.3$, $\xi = -0.5$, and $\xi = -0.7$. The upper index i means that the function $\theta_{cq}(\tilde{\omega})$ is an increasing function and index d means that it is a decreasing function. The maximum frequencies are equal to $\tilde{\omega}_{max} = 8.4$ for $\xi = -0.3$, and $\tilde{\omega}_{max} = 6.0$ for $\xi = -0.5$, and $\tilde{\omega}_{max} = 3.6$ for $\xi = -0.7$.

Now let us turn to the question (II) that have been formulated at the beginning of this section and consider in brief the caustic in BCC and SC lattices in the framework of the Heisenberg model with interaction of a chosen spin and it’s nearest and next nearest neighbors.

The dispersion relations are

$$\begin{gathered}\tilde{\omega}(\mathbf{q}) = 2\{3 - \cos aq_x - \cos aq_y - \cos aq_z\}+ \\ +4\xi\{3 - \cos aq_x \cos aq_y - \cos aq_x \cos aq_z - \cos aq_y \cos aq_z\}\end{gathered} \tag{4}$$

Table 1. Caustic directions in FCC lattice.

ξ	$\tilde{\omega}$	$\theta_{cq}^{\{100\}}(\tilde{\omega})$	$\theta_{cq}^{\{110\}}(\tilde{\omega})$
-0.3	$(7.06; 8.4)$	$(22°; 45°)^d$	$(55°; 90°)^d$
-0.5	$(4.0; 6.0)$	$(0°; 45°)^d$	$(55°; 90°)^d$
-0.7	$(1.58; 2.45)$	$(0°; 45°)^d$	$(73°; 90°)^d$
	$(2.45; 3.6)$	$(0°; 13°)^i$	$(55°; 73°)^d$
			$(0°; 55°)^i$
			$(0°; 16°)^i$

Table 2. Caustic directions in SC lattice.

ξ	$\tilde{\omega}$	$\theta_{cq}^{\{100\}}(\tilde{\omega})$	$\theta_{cq}^{\{110\}}(\tilde{\omega})$
-0.15	$(1.11; 1.48)$	$(17°; 45°)^d$	$(69°; 90°)^d$
	$(1.48; 1.6)$	$(0°; 17°)^d$	$(66°; 69°)^d$
			$(28°; 40°)^i$
			$(0°; 28°)^d$
-0.2	$(0.36; 0.57)$	$(20°; 45°)^d$	$(68°; 90°)^d$
	$(0.57; 0.8)$	$(0°; 20°)^d$	$(61°; 68°)^d$
			$(31°; 47°)^i$
			$(0°; 31°)^d$
-0.24	$(0.018; 0.0375)$	$(21°; 45°)^d$	$(68°; 90°)^d$
	$(0.0375; 0.16)$	$(0°; 21°)^d$	$(57°; 68°)^d$
			$(31°; 52°)^i$
			$(0°; 31°)^d$

for simple cubic and

$$\tilde{\omega}(\mathbf{q}) = 8\left\{1 - \cos\frac{aq_x}{2}\cos\frac{aq_y}{2}\cos\frac{aq_z}{2}\right\} + 2\xi\{3 - \cos aq_x - \cos aq_y - \cos aq_y\} \tag{5}$$

for body centered cubic lattice. The previously relized for FCC lattice analysis of caustics was performed for these dispersion laws as well. Note that the region of possible values of ξ is limited for cubic lattices. For instance, in SC lattices with $\xi < -0.25$ the function $\tilde{\omega}(q)$ becomes negative and decreasing at small values of q for [001] direction. Thus, it is necessary to have $\xi > -0.25$ for a simple cubic lattice. Note that the limit value of ξ is equal to -1 for BCC and FCC lattices for the same reasons. That is why the results of a SC lattices investigation are formulated for $\xi = -0.15$ (far from the critical region), $\xi = -0.2$ (middle region), and $\xi = -0.24$ (close to the critical region). The result is compiled in the Table 2 for simple cubic lattices and in the Table 3 for body centered ones.

The caustic picture is the simplest in the BCC lattices. In this case a single caustic can be observed both in the $\{100\}$ and $\{110\}$ planes. The region of caustic directions becomes practically independent on the parameter ξ but the region of corresponding frequencies shifts to the lower zone with increasing absolute value of ξ. In the case of a simple cubic lattice the caustic picture is more complicated. As for the case of SC lattice, there is one caustic in $\{100\}$ plane, and $\theta_{cq}^{\{100\}}$ is a decreasing function of $\tilde{\omega}$. Moreover $\theta_{cq}^{\{100\}}(\tilde{\omega}_l) = \pi/4$ and $\theta_{cq}^{\{100\}}(\tilde{\omega}_r) = 0$,

Table 3. Caustic directions in BCC lattice.

ξ	$\tilde{\omega}$	$\theta_{cq}^{\{100\}}(\tilde{\omega})$	$\theta_{cq}^{\{110\}}(\tilde{\omega})$
-0.3	$(3.92; 4.51)$	$(0°; 45°)^d$	$(56°; 90°)^d$
-0.5	$(2.0; 2.50)$	$(0°; 45°)^d$	$(56°; 90°)^d$
-0.7	$(0.72; 0.97)$	$(0°; 45°)^d$	$(56°; 90°)^d$

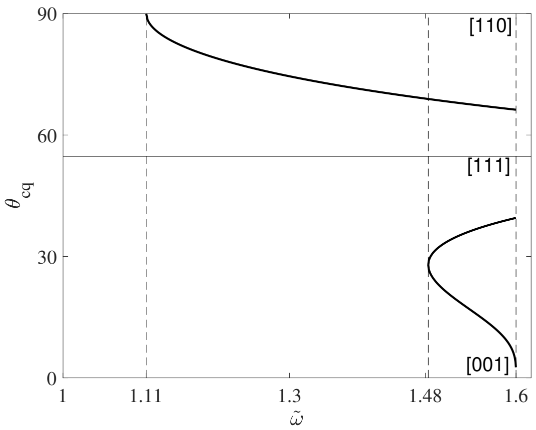

Figure 5. Dependence of caustic directions on magnon frequency ($\tilde{\omega}$) for $\{110\}$ plane in a simple cubic lattice with $\xi = -0.15$.

where $(\tilde{\omega}_l, \tilde{\omega}_r)$ is the caustic frequency region that is determined by the value ξ. The situation in the $\{110\}$ planes is explained easier if the dependence of $\tilde{\omega}_c(\theta_{cq})$ is considered instead of the dependence $\theta_{cq}(\tilde{\omega})$. When θ_{cq} increases from zero to some value θ_1, the caustic frequency decreases from $\tilde{\omega}_{max}$, reaches the minimum and increases up to $\tilde{\omega}_{max}$ at $\theta = \theta_1$. Further, caustics cannot be observed if $\theta_1 < \theta < \theta_2$. When $\theta_2 < \theta < \pi/2$ a caustic exists again and represents a decreasing function of θ. The values of θ_1 and θ_2 are determined by the value ξ. For instance, $\theta_1 \approx 40°$ and $\theta_2 \approx 66°$ if $\xi = -0.3$. The situation is demonstrated in the figure 5, where the caustic picture for $\{110\}$ plane in a SC lattice with $\xi = -0.15$ is shown.

5. Conclusions

Based on Heisenberg exchange model we investigated the spin wave caustics behavior in ferromagnets with cubic lattices. We began our research with an analysis of a well-known material, namely EuS, and then extended the developed method to other cubic lattice ferromagnets. The dependencies of the number of caustic directions on the exchange interaction parameters were investigated in body centered, face-centered and simple cubic ferromagnets. The dependencies of the caustic direction on the magnon frequency are also investigated. It is important that the group velocity vector and the wavevector are noncollinear to each other in cubic lattices, and it is necessary to determine the caustic angle both in the space of wavenumbers and in the space of group velocities. In particular, it was shown that only one caustic can be observed in EuS compound in $\{100\}$ and $\{110\}$ planes when the frequency locates in the specific region. In the $\{100\}$ plane, the caustic direction both in q- and V-spaces rotates from $\pi/4$ to 0 when the frequency changes from 138 to 206 GHz. As for the $\{110\}$ plane, the caustic direction changes from 90° to 55° in q-space, and from 90° to 110° in V-space in the same frequency region.

General results for various lattices and various interactions can be compiled as follows:
(1) Magnon caustics appear at high frequencies for all kinds of lattices at the negative values of ξ.
(2) Depending on the magnon freuency and the value of coupling parameter ξ there can be only one caustic direction in the crystallographic planes, but for ome cases there are several directions. In all considered cases, one of the caustic branches is a decreasing function on frequency. For this branch in the $\{100\}$ plane caustic direction in q-space rotates from [110] to [100], and in the $\{110\}$ plane caustics move from [110] to the direction close to [111].
(3) For FCC lattice three-caustic frequency region exists if the value of ξ is negative and large enough, in particular, for $\xi = -0.7$. For SC lattice this frequency region exists even for small negative ξ. In BCC lattice, only one-caustic-in-one-plane regime can be realized.

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